```
=> s mdl 100907/cn
L14           1 MDL 100907/CN

=> d

L14  ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2006 ACS on STN
RN   139290-65-6  REGISTRY
ED   Entered STN:  28 Feb 1992
CN   4-Piperidinemethanol, α-(2,3-dimethoxyphenyl)-1-[2-(4-
     fluorophenyl)ethyl]-, (αR)- (9CI)  (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN   4-Piperidinemethanol, α-(2,3-dimethoxyphenyl)-1-[2-(4-
     fluorophenyl)ethyl]-, (R)-
OTHER NAMES:
CN   (+)-α-(2,3-Dimethoxyphenyl)-1-[2-(4-fluorophenyl)ethyl]-4-
     piperidinemethanol
CN   (+)-MDL 100907
CN   M 100907
CN   MDL 100907
CN   R-MDL 100907
FS   STEREOSEARCH
MF   C22 H28 F N O3
CI   COM
SR   CA
LC   STN Files:   ADISINSIGHT, ADISNEWS, ANABSTR, BIOSIS, BIOTECHNO, CA,
       CAPLUS, CASREACT, EMBASE, IMSDRUGNEWS, IMSPATENTS, IMSRESEARCH, IPA,
       MEDLINE, PHAR, PROUSDDR, RTECS*, SYNTHLINE, TOXCENTER, USPAT2, USPATFULL
         (*File contains numerically searchable property data)

Absolute stereochemistry.  Rotation (+).
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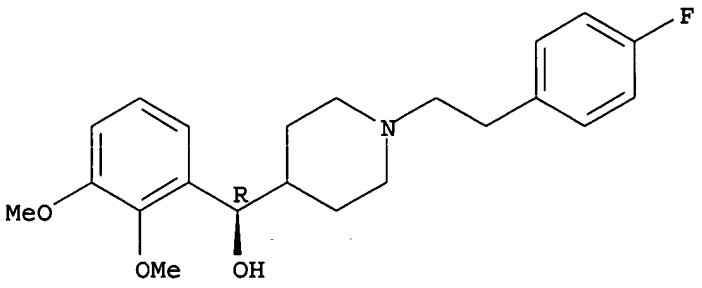


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**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

             187 REFERENCES IN FILE CA (1907 TO DATE)
               3 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
             187 REFERENCES IN FILE CAPLUS (1907 TO DATE)


=> fil caplus
COST IN U.S. DOLLARS                            SINCE FILE      TOTAL
                                                  ENTRY    SESSION
FULL ESTIMATED COST                                7.10     145.10

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)      SINCE FILE      TOTAL
                                                  ENTRY    SESSION
CA SUBSCRIBER PRICE                                0.00      -4.50

FILE 'CAPLUS' ENTERED AT 15:39:18 ON 02 AUG 2006
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FILE COVERS 1907 - 2 Aug 2006 VOL 145 ISS 6
FILE LAST UPDATED: 1 Aug 2006 (20060801/ED)


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=> s l14
L15        187 L14

=> s l15(l)metabol?
         888348 METABOL?
L16           2 L15(L)METABOL?

=> d bib abs hitstr 1-2

L16  ANSWER 1 OF 2  CAPLUS  COPYRIGHT 2006 ACS on STN
AN   1998:313969  CAPLUS
DN   129:49176
TI   Investigation of the CNS penetration of a potent 5-HT2a receptor
     antagonist (MDL 100,907) and an active metabolite (MDL 105,725) using in
     vivo microdialysis sampling in the rat
AU   Scott, Dennis O.; Heath, Timothy G.
CS   Hoechst Marion Roussel, Inc, Kansas City, MO, 64134-0627, USA
SO   Journal of Pharmaceutical and Biomedical Analysis (1998), 17(1), 17-25
     CODEN: JPBADA; ISSN: 0731-7085
PB   Elsevier Science B.V.
DT   Journal
LA   English
AB   MDL 100,907 is a selective 5-HT2a receptor antagonist which is currently
     being developed for the treatment of schizophrenia.  Pharmacokinetic
     studies of MDL 100,907 in rats and dogs show that the drug is well
     absorbed but undergoes extensive first-pass metabolism to an active metabolite
     (MDL 105,725).  The purpose of this study was to determine concns. of MDL
     100,907 and MDL 105,725 in the brain extracellular fluid (ECF) after
     administration of MDL 100,907.  In vivo microdialysis sampling was used to
     determine the brain penetration of both parent (MDL 100,907) and metabolite
     (MDL 105,725).  Animals (n = 3/dose) were given 5 i.v. and 50 mg kg-1 oral
     doses of MDL 100.907.  Brain medial prefrontal cortex (mPFC) ECF concns.
     were determined using microdialysis and plasma levels were determined by
collecting
     blood samples through an indwelling cannula implanted in the jugular vein.
     Dialyzate samples were analyzed using an LC/MS/MS assay.  The data
     presented in this report show that the blood brain barrier (BBB)
     permeability of MDL 100,907 is more than four times (4 +) that of
     MDL 105,725 and that MDL 100,907 does not undergo significant metabolism to
     MDL 105,725 in the brain.  It appears, from the data presented, that MDL
     100,907 is the predominant active species present in the brain at high
```

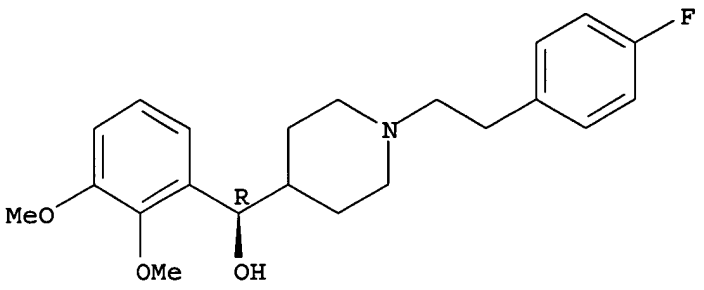
doses.

IT 139290-65-6, MDL 100907
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(CNS penetration of 5-HT2a receptor antagonist MDL 100,907 and active metabolite MDL 105,725)

RN 139290-65-6 CAPLUS

CN 4-Piperidinemethanol, α-(2,3-dimethoxyphenyl)-1-[2-(4-fluorophenyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1997:239223 CAPLUS

DN 126:287509

TI Quantification of a potent 5-HT2a antagonist and an active metabolite in rat plasma and brain microdialyzate by liquid chromatography-tandem mass spectrometry

AU Heath, Timothy G.; Scott, Dennis O.

CS Hoechst Marion Roussel, Kansas City, MO, 64134-0627, USA

SO Journal of the American Society for Mass Spectrometry (1997), 8(4), 371-379
CODEN: JAMSEF; ISSN: 1044-0305

PB Elsevier

DT Journal

LA English

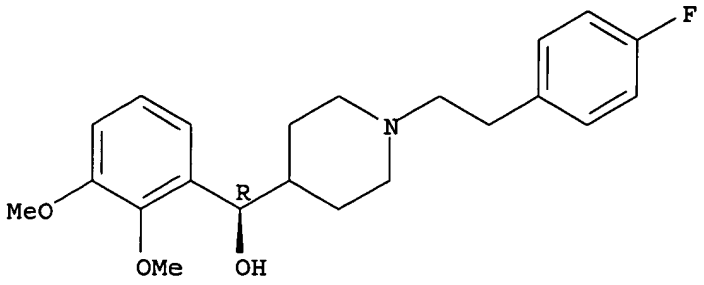
AB A method based on liquid chromatog.-tandem mass spectrometry and microbore column separation was developed for the quantification of a potent 5-HT2a receptor antagonist, MDL 100,907 [(R)-(+)-α-(2,3-dimethoxyphenyl)-1-[2-(4-fluorophenyl)ethyl]-4-piperidinemethanol] (I) and its demethyl metabolite (II) in rat brain extracellular fluid (ECF) following microdialysis sampling. The method was also applied to determining plasma concns. of these compds. The lower limit of quantification (LLQ) for each compound in the microdialysis perfusate is 500 pg/mL, which translates to <7 fmol (injected). The recovery of I and II from the microdialysis probe in brain ECF was 18.5 and 22.7%, resp. The LLQ for each compound in plasma was 1 ng/mL. The inherent selectivity offered by tandem mass spectrometry eliminated chemical noise, thereby improving the detectability of these compds. These methods were used to confirm that I and II penetrated the blood-brain barrier following administration of I to rats and enabled comparison of plasma and brain ECF concns.

IT 139290-65-6, MDL 100907
RL: ANT (Analyte); ANST (Analytical study)
(determination of serotoninergic S2a antagonist MDL 100,907 and its demethyl metabolite in brain extracellular fluid and plasma by liquid chromatog.-mass spectrometry)

RN 139290-65-6 CAPLUS

CN 4-Piperidinemethanol, α-(2,3-dimethoxyphenyl)-1-[2-(4-fluorophenyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



AN 2001:63973 CAPLUS
DN 134:115860
TI Preparation of sulfuric acid mono-[3-({1-[2-(4-fluoro-phenyl)-ethyl]-piperidin-4-yl}-hydroxy-methyl)-2-methoxy-phenyl]ester and analogs for use as serotonin 5HT2A receptor antagonists
IN Bernotas, Ronald; Brown, Paul; Emmons, Gary; King, Chi-Hsin
PA Aventis Pharmaceuticals Inc., USA
SO PCT Int. Appl., 54 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001005764	A2	20010125	WO 2000-US19065	20000713
	WO 2001005764	A3	20011004		
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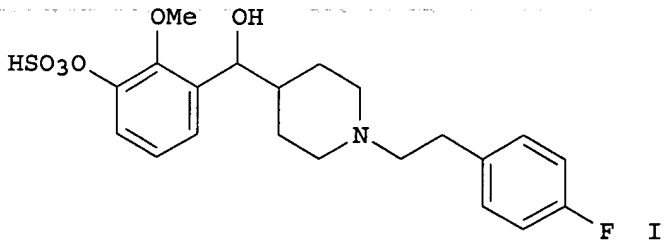
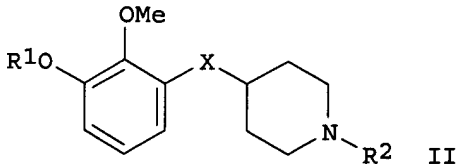
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	CA 2374635	AA	20010125	CA 2000-2374635	20000713
	BR 2000012477	A	20020402	BR 2000-12477	20000713
	EP 1202967	A2	20020508	EP 2000-947304	20000713
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
	JP 2003505374	T2	20030212	JP 2001-511425	20000713
	AU 769484	B2	20040129	AU 2000-60939	20000713
	NZ 516286	A	20040326	NZ 2000-516286	20000713
	ZA 2002000101	A	20030404	ZA 2002-101	20020104
	NO 2002000213	A	20020222	NO 2002-213	20020115
PRAI	US 1999-354704	A2	19990716		
	WO 2000-US19065	W	20000713		

OS MARPAT 134:115860
GI



I



II

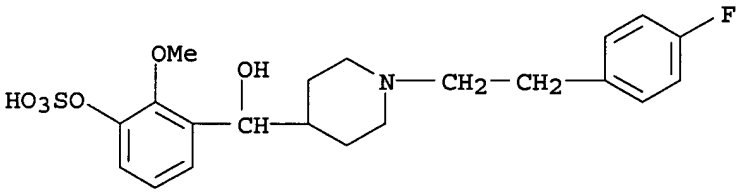
AB Preparation of the title compound I and its analogs II (R1 = H, trialkylsilane,

alkylcarboxy; R2 = (un)substituted arylalkyl, COOR3, H; R3 = alkyl, aryl or arylalkyl; X = CO or CHOR4; R4 = H or alkylcarboxy) is disclosed. Thus, compound I was prepared by combined sulfonation/deacetylation of acetic acid {1-[2-(4-fluorophenyl)-ethyl]-piperidin-4-yl}-(3-hydroxy-2-methoxyphenyl)methyl ester. I is an active metabolite of II (R1 = Me; X = CHOH; R2 = 4-FC6H4CH2CH2) and a method for its preparation and isolation via metabolism is claimed. The title compds. are claimed as serotonin 5HT2A receptor antagonists and as such are useful for the treatment of a number of disease states, e.g. schizophrenia, anxiety, variant angina, anorexia nervosa, cardiac arrhythmias, etc.

IT 321547-54-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); MFM (Metabolic formation); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation); USES (Uses)
(preparation and metabolic formation of the active metabolite sulfuric acid mono[({[fluorophenylethyl]piperidinyl}hydroxymethyl)methoxyphenyl] ester)

RN 321547-54-0 CAPLUS

CN 4-Piperidinemethanol, 1-[2-(4-fluorophenyl)ethyl]-α-[2-methoxy-3-(sulfooxy)phenyl]- (9CI) (CA INDEX NAME)

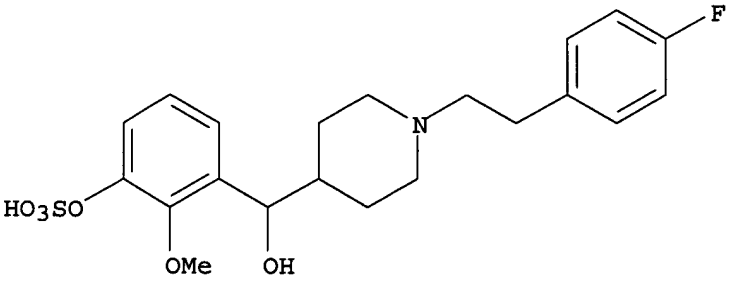


IT 321547-50-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); MFM (Metabolic formation); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(stereoselective preparation and metabolic formation of the active metabolite sulfuric acid mono[({[fluorophenylethyl]piperidinyl}hydroxymethyl)methoxyphenyl] ester)

RN 321547-50-6 CAPLUS

CN 4-Piperidinemethanol, 1-[2-(4-fluorophenyl)ethyl]-α-[2-methoxy-3-(sulfooxy)phenyl]-, (+)- (9CI) (CA INDEX NAME)

Rotation (+).



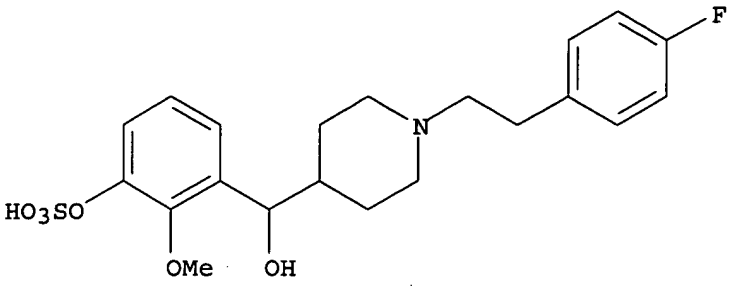
IT 321547-58-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); MFM (Metabolic formation); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation); USES (Uses)

(stereoselective preparation and metabolic formation of the active metabolite sulfuric acid mono[({[fluorophenylethyl]piperidinyl}hydroxymethyl)methoxyphenyl] ester)

RN 321547-58-4 CAPLUS

CN 4-Piperidinemethanol, 1-[2-(4-fluorophenyl)ethyl]-α-[2-methoxy-3-(sulfooxy)phenyl]-, (-)- (9CI) (CA INDEX NAME)

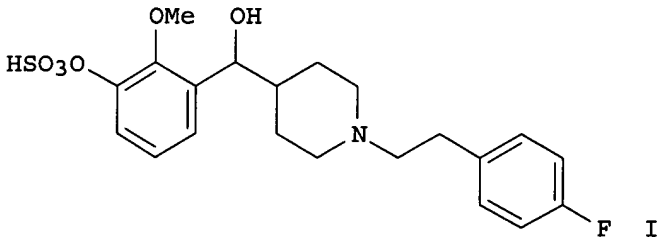
Rotation (-).



AN 2002:790226 CAPLUS
DN 137:310813
TI Preparation of sulfuric acid mono-[3[[1-[2-(4-fluorophenyl)ethyl]-piperidin-4-yl]hydroxymethyl]-2-methoxyphenyl]ester and enantiomers as 5HT2A antagonists.
IN Bernotas, Ronald Charles; Brown, Paul Wayne; Emmons, Gary Thomas; King, Chi-hsin Richard
PA Aventis Pharmaceuticals Inc., USA
SO U.S., 19 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6465490	B1	20021015	US 2000-615246	20000713 <--
	US 2003087932	A1	20030508	US 2002-200821	20020722
	US 6716986	B2	20040406		
	US 2004152900	A1	20040805	US 2004-760515	20040120
PRAI	US 1999-198215P	P	19990716		
	US 2000-615246	A3	20000713		
	US 2002-200821	A3	20020722		

OS CASREACT 137:310813
GI



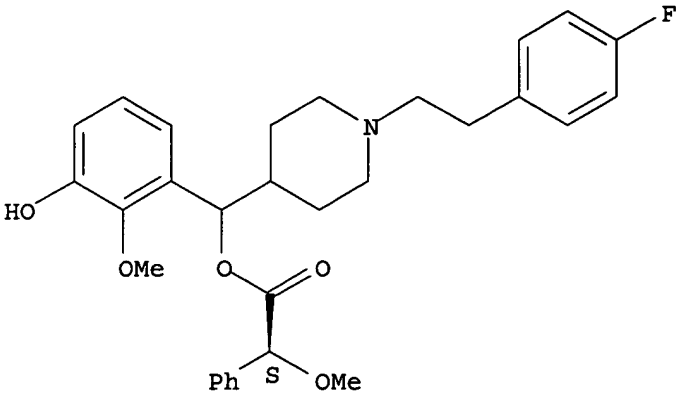
I

AB Title compds. I were prepared Thus, acetic acid [1-[2-(4-fluorophenyl)ethyl]piperidin-4-yl](3-hydroxy-2-methoxyphenyl)methyl ester (preparation given) was heated at 45° with SO3.pyridine in MeCN for 18 h; H2O, MeOH, and K2CO3 were added followed by 12 h reflux to give sulfuric acid mono-(+)-[3[[1-[2-(4-fluorophenyl)ethyl]piperidin-4-yl]hydroxymethyl]-2-methoxyphenyl] ester. Title compds. were shown to penetrate the blood-brain barrier.

RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 1 OF 10 REGISTRY COPYRIGHT 2006 ACS on STN
RN 321547-55-1 REGISTRY
ED Entered STN: 13 Feb 2001
CN Benzeneacetic acid, α-methoxy-, [1-[2-(4-fluorophenyl)ethyl]-4-piperidinyl](3-hydroxy-2-methoxyphenyl)methyl ester, (αS)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C30 H34 F N O5
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPAT2, USPATFULL

Absolute stereochemistry.



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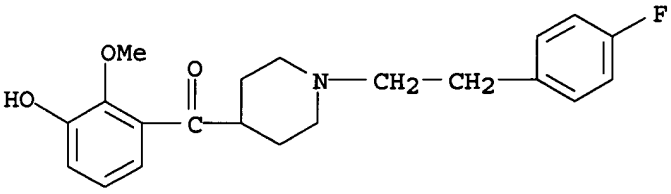
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L8 ANSWER 2 OF 10 REGISTRY COPYRIGHT 2006 ACS on STN
RN 321547-53-9 REGISTRY
ED Entered STN: 13 Feb 2001
CN Methanone, [1-[2-(4-fluorophenyl)ethyl]-4-piperidinyl](3-hydroxy-2-methoxyphenyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C21 H24 F N O3
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPAT2, USPATFULL



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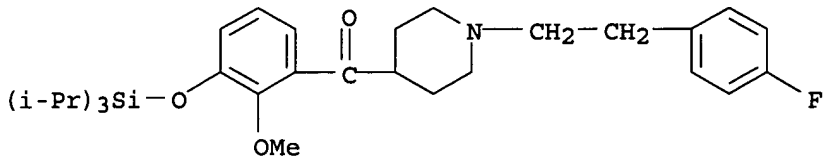
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L8 ANSWER 3 OF 10 REGISTRY COPYRIGHT 2006 ACS on STN
RN 321547-52-8 REGISTRY

ED Entered STN: 13 Feb 2001
CN Methanone, [1-[2-(4-fluorophenyl)ethyl]-4-piperidinyl][2-methoxy-3-[[tris(1-methylethyl)silyl]oxy]phenyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C30 H44 F N O3 Si
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPAT2, USPATFULL



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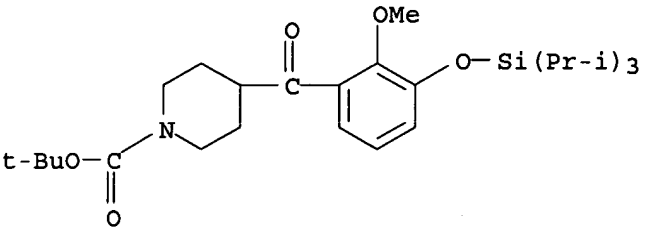
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L8 ANSWER 4 OF 10 REGISTRY COPYRIGHT 2006 ACS on STN
RN 321547-51-7 REGISTRY
ED Entered STN: 13 Feb 2001
CN 1-Piperidinecarboxylic acid, 4-[2-methoxy-3-[[tris(1-methylethyl)silyl]oxy]benzoyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C27 H45 N O5 Si
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPAT2, USPATFULL



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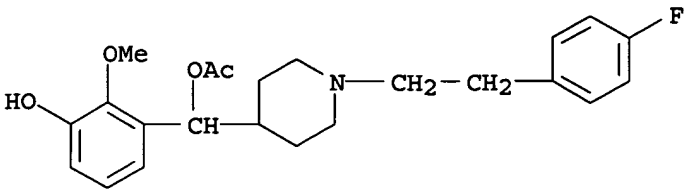
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L8 ANSWER 5 OF 10 REGISTRY COPYRIGHT 2006 ACS on STN
RN 321547-49-3 REGISTRY
ED Entered STN: 13 Feb 2001
CN 4-Piperidinemethanol, 1-[2-(4-fluorophenyl)ethyl]-α-(3-hydroxy-2-methoxyphenyl)-, monoacetate (ester) (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C23 H28 F N O4
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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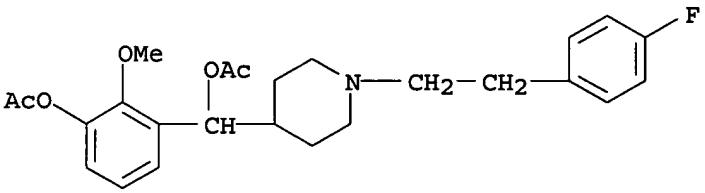
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L8 ANSWER 6 OF 10 REGISTRY COPYRIGHT 2006 ACS on STN
RN 321547-48-2 REGISTRY
ED Entered STN: 13 Feb 2001
CN 4-Piperidinemethanol, α-[3-(acetyloxy)-2-methoxyphenyl]-1-[2-(4-fluorophenyl)ethyl]-, acetate (ester) (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C25 H30 F N O5
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L8 ANSWER 7 OF 10 REGISTRY COPYRIGHT 2006 ACS on STN
RN 321547-47-1 REGISTRY
ED Entered STN: 13 Feb 2001
CN Benzeneacetic acid, α-methoxy-, [1-[2-(4-fluorophenyl)ethyl]-4-piperidinyl][2-methoxy-3-[[tris(1-methylethyl)silyl]oxy]phenyl]methyl ester, (αS)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C39 H54 F N O5 Si
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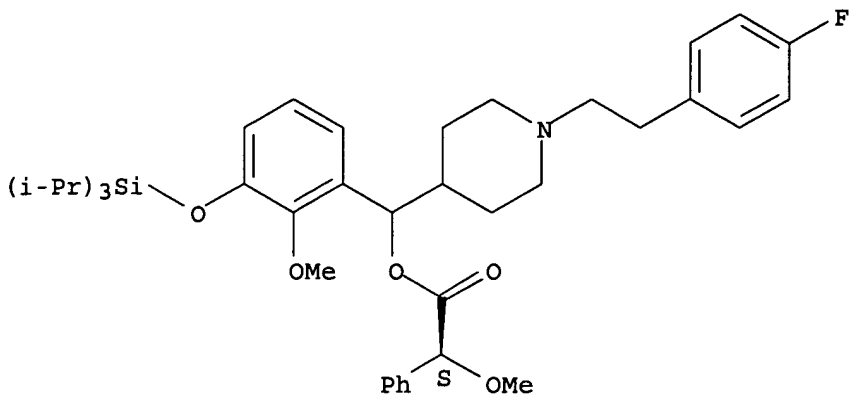
LC STN Files: CA, CAPLUS, CASREACT, USPAT2, USPATFULL

Absolute stereochemistry.



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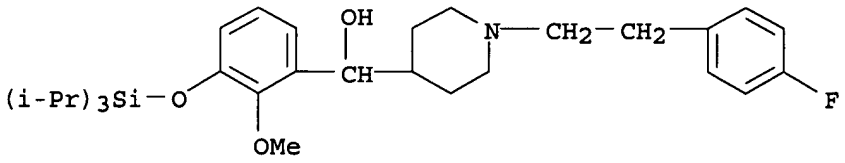
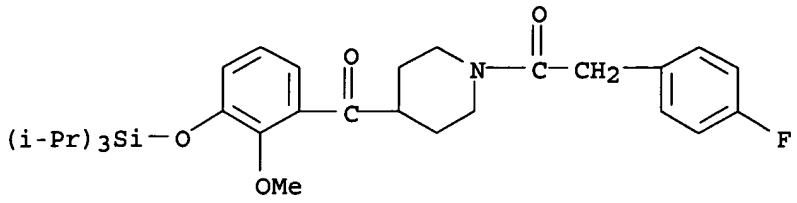
LC STN Files: CA, CAPLUS, CASREACT, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L8 ANSWER 9 OF 10 REGISTRY COPYRIGHT 2006 ACS on STN
RN 321547-45-9 REGISTRY
ED Entered STN: 13 Feb 2001
CN Piperidine, 1-[(4-fluorophenyl)acetyl]-4-[2-methoxy-3-[[tris(1-methylethyl)silyl]oxy]benzoyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C30 H42 F N O4 Si
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPAT2, USPATFULL

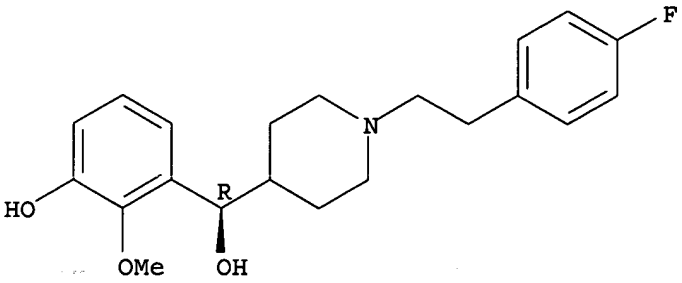


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L8 ANSWER 10 OF 10 REGISTRY COPYRIGHT 2006 ACS on STN
RN 189192-18-5 REGISTRY
ED Entered STN: 22 May 1997
CN 4-Piperidinemethanol, 1-[2-(4-fluorophenyl)ethyl]-α-(3-hydroxy-2-methoxyphenyl)-, (αR)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 4-Piperidinemethanol, 1-[2-(4-fluorophenyl)ethyl]-α-(3-hydroxy-2-methoxyphenyl)-, (R)-
OTHER NAMES:
CN (+)-MDL 105725
CN MDL 105725
FS STEREOSEARCH
MF C21 H26 F N O3
SR CA
LC STN Files: BIOSIS, CA, CAPLUS, CASREACT, USPAT2, USPATFULL

Absolute stereochemistry. Rotation (+).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)
9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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     (FILE 'HOME' ENTERED AT 15:31:08 ON 02 AUG 2006)

     FILE 'CAPLUS' ENTERED AT 15:31:18 ON 02 AUG 2006
L1             1 S US6465490/PN
L2           ANALYZE L1 1 RN :      20 TERMS

     FILE 'REGISTRY' ENTERED AT 15:31:36 ON 02 AUG 2006
L3            20 S L2
L4            14 S L3 AND PIPERIDIN?
L5             3 S L4 AND SULFO?
L6            11 S L4 NOT L5
L7             1 S  139290-70-3
L8            10 S L6 NOT L7

     FILE 'CAPLUS' ENTERED AT 15:33:18 ON 02 AUG 2006
L9             9 S L8
L10            3 S L9 AND METABO?

     FILE 'REGISTRY' ENTERED AT 15:35:05 ON 02 AUG 2006
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